Octane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 312

Global applicability domain: Inside

Local applicability domain index: 5.15e-01

Confidence level: 6.52e-01

Nearest Neighbors from the Training Set

Image not found
Dibenzofuran
Measured: 1510
Predicted: 14.2

Image not found
1-Ethenoxy-2-ethylhexane
Measured: 603
Predicted: 284

Image not found
Carbazole
Measured: 170
Predicted: 10.1

Image not found
Cyclohexane
Measured: 83.2
Predicted: 59.1

Image not found
Methylcyclohexane
Measured: 186
Predicted: 233